Spin in a variable magnetic field: the adiabatic approximation
Spin dans un champ magnétique variable: l'approximation adiabatique

M. S. Marinov[a,b] and Eugene Strahov[a]
(a) *Physics Dept., Technion-Israel Institute of Technology Haifa, 32000 Israel*
(b) *LGCR, Université Pierre et Marie Curie - CNRS URA 7698 4, Place Jussieu, 75005 Paris, France*

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Abstract

The problem of spin precession in a time-dependent magnetic field is considered in the adiabatic approximation where the field direction or the angular velocity of its rotation is changing slowly. The precession angles are given by integrals in a way similar to the semi-classical approximation for the Schrödinger equation.

Keywords: magnetic spin precession, adiabatic approximation

Résumé. Le problème de la précession du spin dans un champ magnétique variable est envisagé selon l'approximation adiabatique dans laquelle la direction du champ où la vitesse de sa rotation varie lentement. Les angles de la précession sont donnés par quadratures de manière similaire à l'approximation semi-classique de l'équation de Schrödinger.

Mots clés: precéssion magnétique du spin, approximation adiabatique

Version française abrégée

Le problème de la précession du spin dans un champ magnétique variable a été résolu explicitement pour deux cas particuliers importants (Landau and Lifshitz 1974, Sect. 114): (i) le champ magnétique ne change pas de direction, (ii) le champ de valeur constante tourne autour d'un axe donné à une vitesse angulaire constante. En outre, des solution analytiques sont obtenues pour certaines variations du champ (cf. Rosenfeld *et al.* 1996). La présente étude a pour but de présenter une solution approchée de l'équation de Bloch (1) décrivant la précession du spin. L'approximation est valable si la direction du champ ou de sa vitesse change adiabatiquement; le résultat principal est énoncé par l'équation (16).

Nous considérons l'équation de Bloch dans le cas où la dépendance du champ magnétique $\mathbf{B}(t)$ de temps t est arbitraire. La solution fondamentale est donnée par une matrice unitaire $U(t, t_0)$ satisfaisant l'équation (3). Cette matrice peut être écrite en termes de deux fonctions complexes (ξ, η), qui satisfont aux équations différentielles (5). Des équations de ce type et des solutions approchées ont été considerées précedémment. Le problème peut être réduit à celui d'un oscillateur a fréquence variable et complexe, eq. (7). Il est à noter que le carré de la fréquence d'oscillation dans l'eq. (7) est une constante réele positive pour les cas simples, mais s'avère être généralement complexe. C'est pourquoi la méthode traditionelle WKBJ ne peut être appliquée directement.

Dans le but de trouver une bonne approximation, la matrice U dans l'eq.(9) est décrite par une rotation d'un angle 2α autour de la vecteur unitaire $\mathbf{n} = (\sin\gamma\cos\delta, \sin\gamma\sin\delta, \cos\gamma)$. Le problème consiste en recherche de la dépendance temporelle des trois angles (α, γ, δ) à partir des équations différentielles (11)-(13).

L'hypothèse cruciale, qui simplifie le problème, est que l'evolution de γ est *très lente*. En d'autres termes, nous supposons que le vecteur $\mathbf{n}$ varie adiabatiquement. Les équations résultantes sont integrées immediatement par quadratures, eq. (16). Il est remarquable que pour les deux cas mentionnés dans le premier paragraphe, l'approximation est exacte, puisque soit (i) $B_\perp \equiv 0$, l'axe de rotation est toujours aligné sur le champ, soit (ii) $\dot{\varphi}, B_z$ et $B_\perp$ sont fixes, de sorte que l'angle entre le champ et l'axe est preservé, ainsi que l'angle γ.

L'approximation edt effective sous deux conditions alternatives: soit (i) la direction du champ $\mathbf{B}$, ou (ii) la direction du vecteur $(\dot{\mathbf{B}} \times \mathbf{B})$, varient lentement autour d'un vecteur $\mathbf{e}$. Dans les deux cas, le vecteur $\mathbf{e}$ indique l'axe z pour le rèpere approprié et pour le choix des paramètres de rotation dans l'équation (9).

La forme de la solution (16) obtenue ressemble à l'approximation semi-classique (ou eikonale) appliquée à la diffusion à haute energie, pour laquelle le potentiel de diffusion était supposé être une fonction d'espace à variation lente.

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The problem of spin precession in variable magnetic field is fundamental for the theory of nuclear magnetic resonance(Abragam 1961). Its explicit solution is known for two important particular cases (Landau and Lifshitz 1974, Sect. 114): i) the magnetic field does not change its direction, ii) the field has a constant magnitude and is precessing around a given axis with a constant angular velocity. Besides, analytical solutions have been obtained for a number of special field shapes (Rosen and Zener 1932, Bambini and Berman 1981, Silver *et al.* 1985, Rosenfeld *et al.* 1996).

As soon as one deals with the Cauchy problem for two coupled linear first-order differential equations, or equivalently, with a second-order equation, an adiabatic approximation may be employed, similarly to the standard semi-classical approach to the Schrödinger equation. An adiabatic approximation for the Bloch equation was the purpose of the present work, and the result is presented in Eq.(16). The key to the desired approximation is a proper group-theoretical parametrization in Eqs.(9-10), which enables one to handle complexities specific to the problem.

The spinor wave function of a neutral spin-$\frac{1}{2}$ particle satisfies the Bloch equation,

$$id\psi/dt = (\mathbf{B} \cdot \sigma)\psi, \tag{1}$$

where $\mathbf{B} = (B_x, B_y, B_z) \equiv \mu\mathcal{B}(t)$, $\mathcal{B}(t)$ is the variable magnetic field vector, μ is the particle magnetic moment, and σ are the Pauli matrices. The fundamental solution of Eq. (1) is given by a unitary 2×2 matrix U,

$$\psi(t) = U(t, t_0)\psi(t_0), \tag{2}$$

$$i\partial U/\partial t = (\mathbf{B} \cdot \sigma)U, \quad U(t_0, t_0) = I. \tag{3}$$

(Here I is the unit matrix.) Two complex functions (ξ, η) are used to represent U,

$$U = \begin{pmatrix} \xi e^{-i\beta} & \bar{\eta} e^{-i\beta} \\ -\eta e^{i\beta} & \bar{\xi} e^{i\beta} \end{pmatrix}; \quad \beta = \int_{t_0}^{t} B_z(\tau) d\tau. \tag{4}$$

In view of Eq. (3), these functions satisfy the following equations,

$$i\dot{\xi} = -b\eta, \quad i\dot{\eta} = -\bar{b}\xi, \quad |\xi|^2 + |\eta|^2 = 1. \tag{5}$$

where

$$b \equiv (B_x - iB_y)e^{2i\beta} = B_\perp e^{2i\beta - 2i\varphi}, \quad B_\perp^2 = \mathbf{B}^2 - B_z^2, \quad \tan 2\varphi = B_y/B_x. \tag{6}$$

Equations of this type and various approximations were considered previously (e.g. by Popov 1962, Marinov and Popov 1979, Rosenfeld *et al.* 1996). The problem may be further reduced to that for an oscillator with a variable (complex) frequency,

$$\ddot{f} + \Omega^2(t) f = 0, \quad f \equiv b^{-1/2}\xi, \tag{7}$$

where

$$\Omega^2 = B_\perp^2 + \omega^2 + i\dot{\omega},$$
$$\omega \equiv -i\dot{b}/2b = B_z - \dot{\varphi} - \frac{i}{4}\frac{d}{dt}\log B_\perp^2, \tag{8}$$

i.e. $2\dot{\varphi} = (B_x\dot{B}_y - \dot{B}_x B_y)/B_\perp^2$ is the angular velocity of the field rotation around the z-axis. Note that Ω^2 is a real positive constant for the cases presented in the textbook, but is complex in general. Therefore the standard WKBJ method cannot be applied to Eq. (7) directly.

A consistent adiabatic approximation for the problem concerned was proposed by Bender and Papanicolaou 1988 and further developed by Papanicolaou 1988. It was assumed that the field time dependence was slow, i.e. the specific variation time T was large, and an expansion in powers of $1/T$ was constructed. An alternative approach, based upon the Magnus expansion, was presented by Klarsfeld and Oteo 1992. Unlike the above mentioned (and a number of other) works, we do not assume a slow time dependence of the field. In particular, the result given below is *exact* for the field rotation with an arbitrarily high (but stable) angular velocity. Actually, we

employ geometrical arguments, which were previously developed for the adiabatic approximation by Nakagawa 1987. With all that, to the best of our knowledge, the result given in Eqs. (9), (16) was never published before.

The complex equations (5) are equivalent to real equations for angles which appear when U is treated as the spinor representation of the rotation group. Let us write U as a product of two matrices representing rotations,

$$U \equiv R_z(\alpha_1)R_n(\alpha), \quad R_n = I\cos\alpha - i(\mathbf{n}\cdot\sigma)\sin\alpha. \tag{9}$$

Here matrix $R_z(\alpha_1)$ has the diagonal elements $(e^{i\alpha_1}, e^{-i\alpha_1})$ only and represents the rotation around the z-axis, and $R_n(\alpha)$ represents a rotation by an angle 2α around the direction of a unit vector $\mathbf{n} = (\sin\gamma\cos\delta, \sin\gamma\sin\delta, \cos\gamma)$. The factor containing $\alpha_1(t)$ transforms the system to a rotating frame. The time dependence of α_1 is chosen in such a way as to make the variation of $\mathbf{n}$ slow. Setting

$$\alpha_1 = -\varphi + \delta/2, \tag{10}$$

we get the following differential equations for the angles (α, γ, δ),

$$\dot\alpha\sin\gamma = \nu\sin(2\gamma - \gamma_0), \tag{11}$$

$$\dot\gamma\tan\alpha = 2\nu\sin(\gamma_0 - \gamma), \tag{12}$$

$$\dot\delta\sin\gamma = 2\nu\sin(\gamma_0 - \gamma), \tag{13}$$

where the new notations are

$$\nu(t) = \sqrt{\dot\varphi^2 - 2\dot\varphi B_z + \mathbf{B}^2}, \quad \cot\gamma_0(t) = (\dot\varphi - B_z)/B_\perp. \tag{14}$$

The initial conditions corresponding to (3) are

$$\alpha(t_0) = 0, \quad \gamma(t_0) = \gamma_0(t_0), \quad \delta(t_0) = \varphi(t_0). \tag{15}$$

The starting precession velocity of $\mathbf{n}$, as given by Eqs. (12),(13), is vanishing, and the crucial assumption is that it is small for all t. In the other words, we assume that the vector $\mathbf{n}$ is moving adiabatically. In contrast to the standard adiabatic approximation, $\mathbf{n}$ does not coincide with the field direction if its change is rapid. As seen from Eq. (14), $\mathbf{n}$ takes a position intermediate between $\mathbf{B}$ and its instantaneous rotation axis $(\dot{\mathbf{B}} \times \mathbf{B})$. The approximate solution of (11)-(13) is

$$\alpha(t, t_0) = \int_{t_0}^{t} \nu(\tau)d\tau, \quad \gamma(t, t_0) \equiv \gamma_0(t), \quad \delta(t, t_0) \equiv \varphi(t_0). \tag{16}$$

For two cases mentioned in the first paragraph the approximation is exact, since either i) $B_\perp = 0$, so $\gamma_0 \equiv 0$, or ii) $\dot\varphi, B_z$, and $B_\perp$ are fixed, so γ_0 is a constant too.

In order to estimate the accuracy of the approximation, let us assume that $\dot\gamma_0$ is small and $\gamma \approx \gamma_0$. Respectively, equation (12) is linearized and solved explicitly

$$\dot\gamma \approx 2(\gamma_0 - \gamma)\dot\alpha\cot\alpha,$$

$$\gamma(t, t_0) \approx \gamma_0(t) + \left[\int_{t_0}^{t} \dot\gamma_0(\tau)\sin^2\alpha(\tau, t_0)d\tau\right] / \sin\alpha^2(t, t_0), \tag{17}$$

where α is given by (16). The approximation is effective under two alternative conditions: either (i) the field direction, or (ii) the direction of the vector $(\dot{\mathbf{B}} \times \mathbf{B})$, is changed slowly around a fixed vector $\mathbf{e}$. In both cases, the vector $\mathbf{e}$ indicates the z axis for the appropriate coordinate system and the choice of the rotation parameters in Eq. (9). A remarkable case is that of a fastly rotating field, where $\dot{\varphi} \gg B_\perp$, and $|\cot\gamma_0| \gg 1$. As a result, the deviation of $\mathbf{n}$ from the z direction is small, even if the field rotation is not stationary. The obtained form of the solution (16) resembles the semi-classical and the eikonal approximation to the high-energy scattering (Landau and Lifshitz, 1974, Sect. 131), since it is valid if $\dot{\nu} \ll \nu^2$.

The validity of our approximation was checked by comparing it with the exact result for a field where the analytical solution was obtained by Rosen and Zener 1932. That field has a constant x-component and a pulse in the y-direction,

$$\mathbf{B}(t) = \frac{1}{T}\left(\beta_0, \frac{\zeta}{\cosh(t/T)}, 0\right), \tag{18}$$

where β_0 and ζ are constant dimensionless parameters. Assuming that the initial state was polarized to the x-axis, the spin-flip probability W was calculated in the time asymptotics, i.e. $t, |t_0| \gg T$. In the limit of $\beta_0 \to \infty$, corresponding to a large T for a fixed background field, the exact and the approximate solutions coincide,

$$W = \zeta^4/\beta_0^2 + O(\beta_0^{-3}). \tag{19}$$

Moreover, the numerical calculations showed that the relative error of our approximation in W is less than 1% for all values of $\beta_0 \geq 1.5$ and $\zeta \geq 1$.

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